

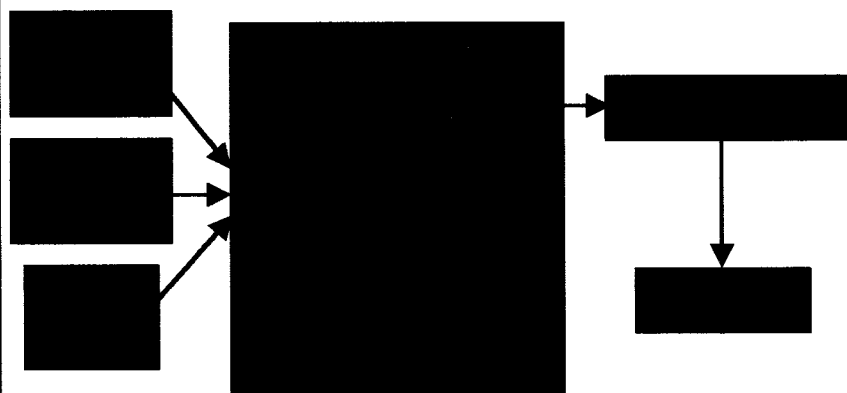
sp³s* and sp³d⁵s*
Tight-binding Parameter Sets for
GaAs, AlAs, InAs,
GaSb, AlSb, InSb,
GaP, AlP, InP
for Quantum Dot Simulations

Gerhard Klimeck*, R. Chris Bowen, and Timothy B. Boykin#
Jet Propulsion Laboratory, California Institute of Technology
#University of Alabama in Huntsville

*Email: gekco@jpl.nasa.gov
Phone: (818) 354 2182
Web: <http://hpc.jpl.nasa.gov/PEP/gekco>

Revolutionary Computing and Sensing are Enabled by Nanoelectronics

4 Basic NASA Missions:
Enabled by Technology



Example NASA Mission Requirements:

- Autonomous spacecraft
 - In-situ data analysis
 - On-board image processing
- => Beyond existing system technology

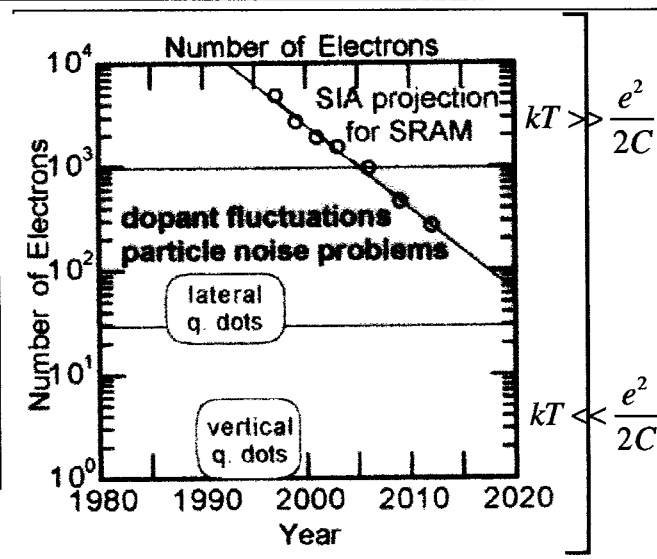
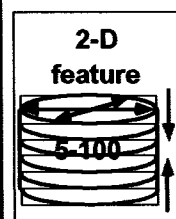
Device/System Requirements:

- Low power and weight, however massive computing and sensing
 - Radiation hard devices
- => Beyond existing device technology

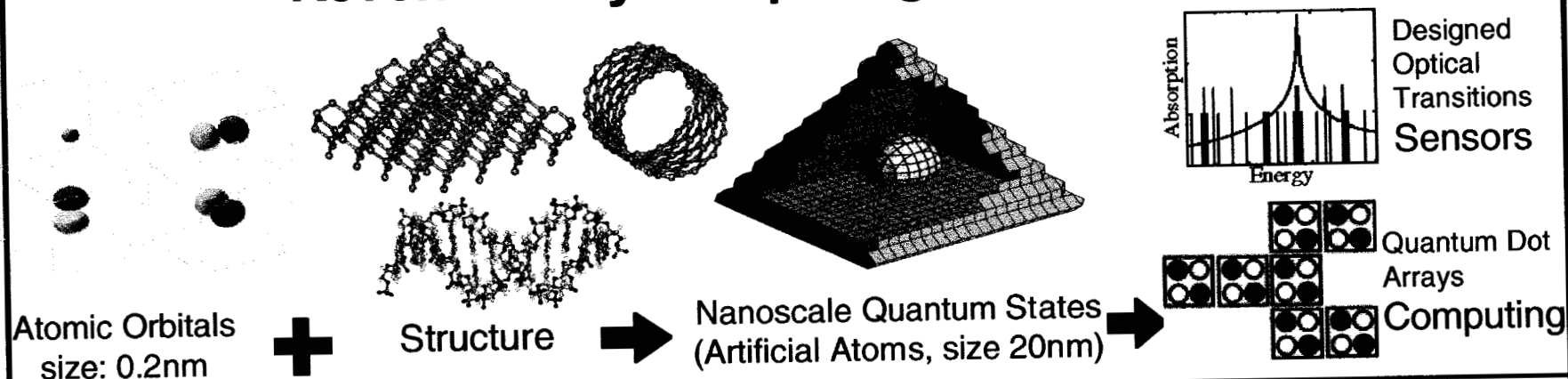
Nanoelectronics:

- Don't fight, **utilize** quantum behavior:
 - Quantized charge
 - Quantized energy
 - Artificial Atoms & Molecules
 - Custom optical transitions
 - New computation architectures
- => Bottom-up 3-D, atomistic device simulation

Another
Look at
Moore's
Law



Quantum Dot Simulation for Revolutionary Computing and Sensing



Opportunity:

- Nanoscale electronic structures can be built!
=> Artificial Atoms / Molecules

Problem:

- The design space is huge: choice of materials, compositions, doping, size, shape.

Approach:

- Deliver a 3-D atomistic simulation tool
- Enable analysis of arbitrary crystal structures, atom compositions and bond/structure configurations.

NASA Relevance:

- 2-5 μ m Lasers and detectors
- High density, low power computation (logic and memory)
- Life signature biosensors

Impact:

- Low cost development of revolutionary technology.
- Narrow empirical/experimental search space

Collaborators:

- Ames, University of Alabama-Huntsville, Purdue

Global Optimization for Microelectronic Device Design

Genetically Engineered NanoElectronic Structures: GENES

Objective:

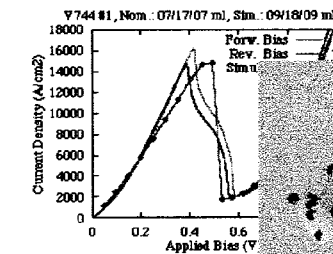
- ¥ Optimize and synthesize electronic devices
- ¥ Limit and focus number of experiments needed to produce design.

Approach:

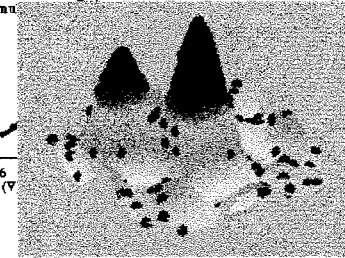
- ¥ Use existing electromagnetic and electronic structure modeling codes
- ¥ Apply genetic algorithm for global optimization
- ¥ Use massively parallel platforms

Impact:

- ¥ Enable device optimization for microelectronic-based missions.
- ¥ Near Term:
 - ¥ Optimize devices.
- ¥ Long Term:
 - ¥ Provide instrument-system level optimization



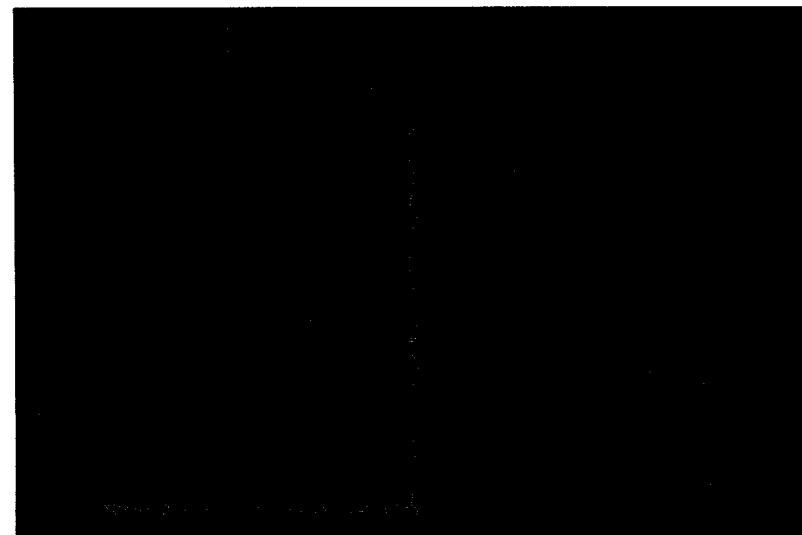
Specification



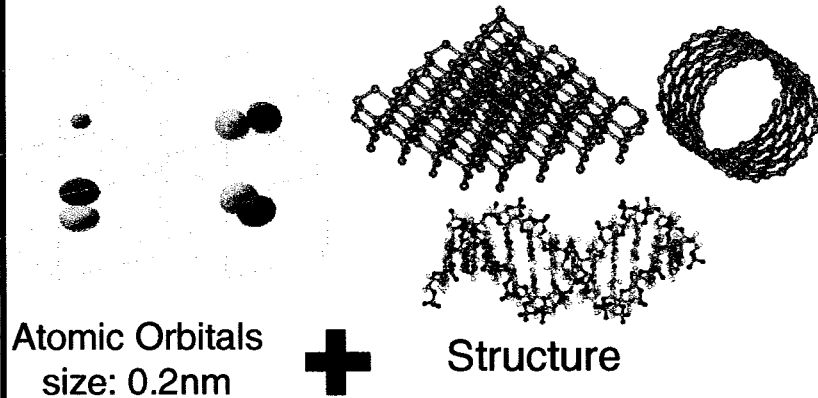
Design/
Synthesis



Fabrication



Mapping of Orbitals to Bulk Bandstructure

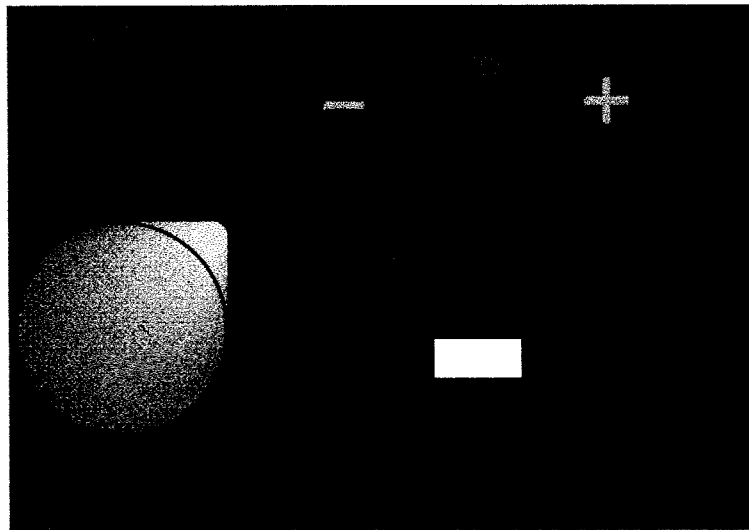


Bulk Semiconductors are described by:

- Conduction and valence bands, bandgaps (direct, indirect), effective masses
- 10-30 physically measurable quantities

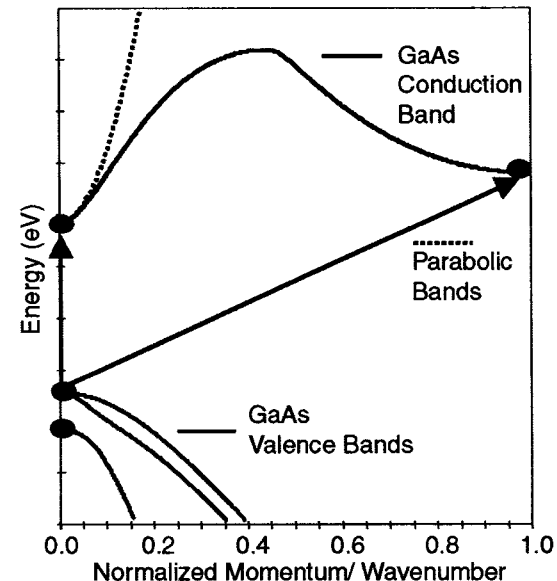
Tight Binding Models are described by:

- Orbital interaction energies.
- 15-30 theoretical parameters



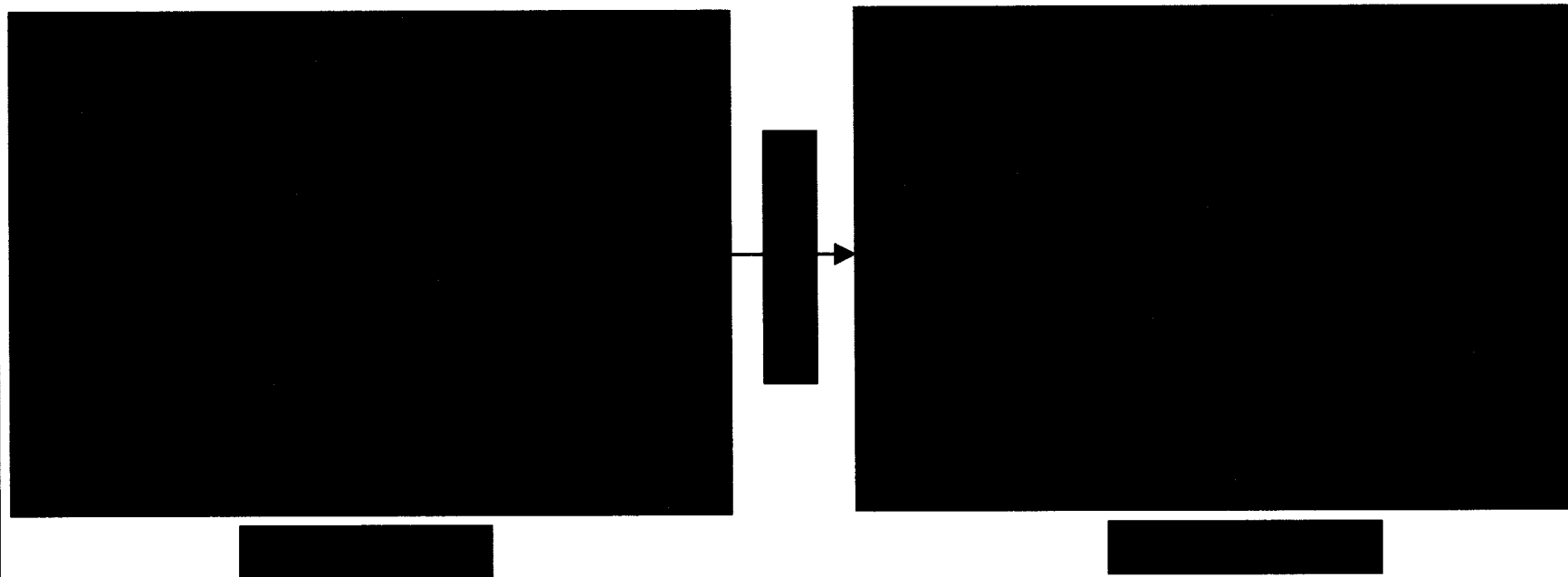
15-30 theoretical interaction energies

High
Dimensional
Fitting
Problem



10-30 data points of bands and masses

Basic Genetic Algorithm



¥Genetic algorithm parameter optimization is based on:

- ¥Survival of good parameter sets
- ¥Evolution of new parameter sets
- ¥Survival of a diverse population

¥Optimization can be performed globally, rather than locally.

Basic Evolution Operations

¥Each set (S_i) consists of several parameters (P_j)

¥The parameters P_j can be of different kinds: real, integers, symbols, .

Gross Exploration



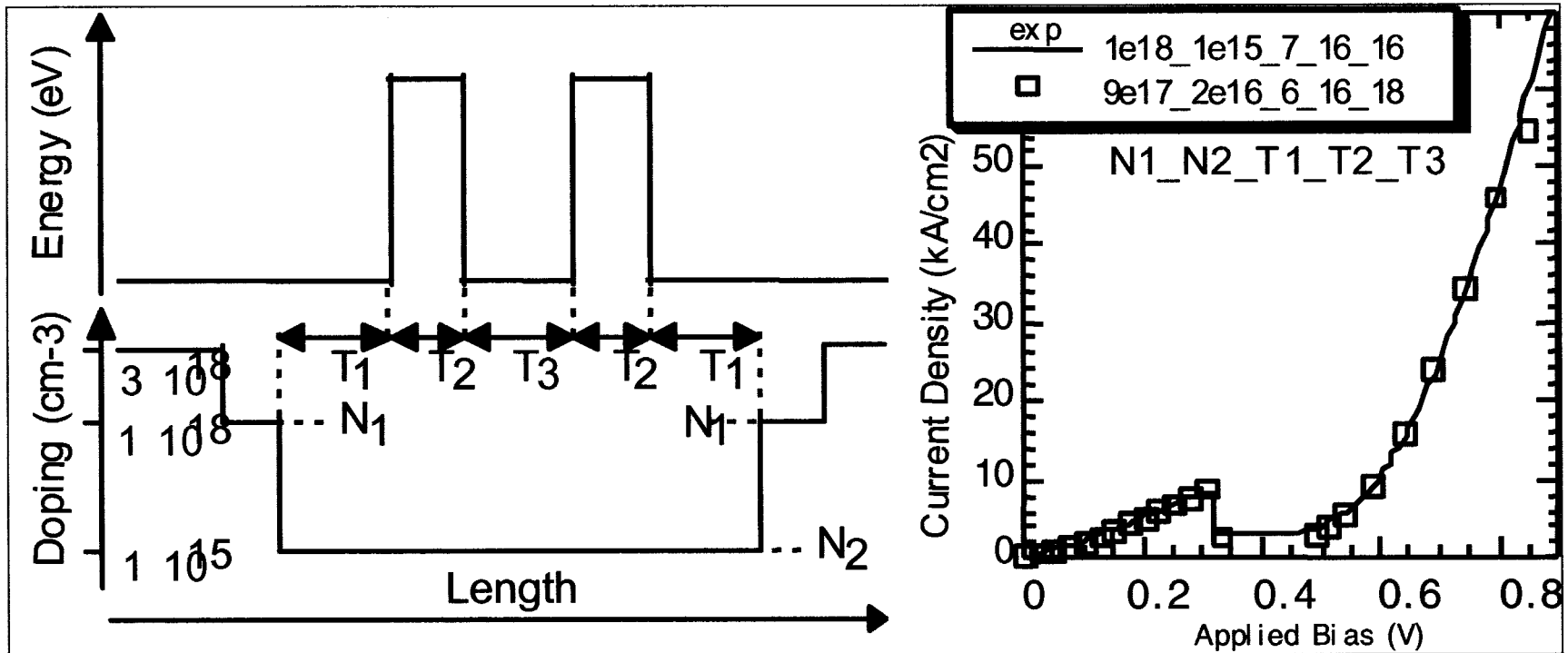
¥Crossover explores different combinations of existing genes.

Fine Tuning



¥Creation of new gene values.

GENES - RTD Structural Analysis



¥Allow genetic algorithm to vary 5 different structural parameters:

¥3 Thicknesses: well, barrier, spacer

¥2 Dopings: low doped spacer, unintentional doping in center

¥Start from random population of 5 parameters.

¥Well width is larger than nominal.

¥No intentional doping is larger than nominal.

RTD Synthesis/Analysis CPU Requirements

¥Single current-voltage characteristic in a simple model:

¥30 minutes on a single CPU

¥Population: 200

¥Replacement: 63 / generation

¥Approximate number of Genes evaluated: 1000

¥Original distributions:

¥ N_1 in $[1 \times 10^{17}, 1 \times 10^{19}]$, N_2 in $[1 \times 10^{14}, 1 \times 10^{16}]$.

¥ T_1 in $[10, 30]$, T_2, T_3 in $[6, 26]$

¥Total CPU time:

¥500hrs on one CPU or

¥8hrs on 64 CPUs

¥Optimization surface is not smooth!

¥Compare to an exhaustive search of $20 \times 20 \times 20 \times 30 \times 30 = 72,000$ combinations => 36,000 hrs

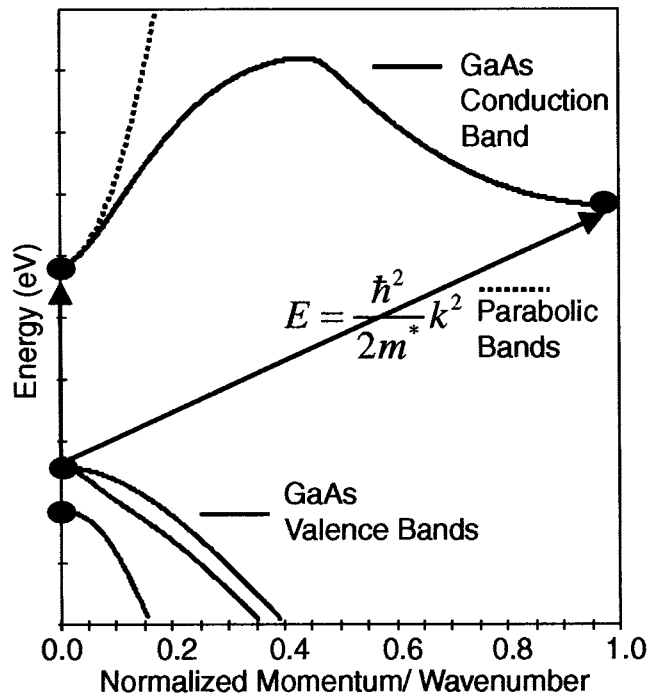
¥Have NOT compared to a line search.

What is known about Bulk Bandstructure?

$$(H_{el} + V_{atomic} + E)\Psi = 0$$

$$H_{el} \propto \nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$$

$$\Psi(r, E) = \Psi_0 e^{ikr} \text{ with dispersion } E(k)$$



Bandstructure describes the propagation of plane waves in a material.

Need to solve Schrödinger Equation

¥ V_{atomic} includes effects of core atoms

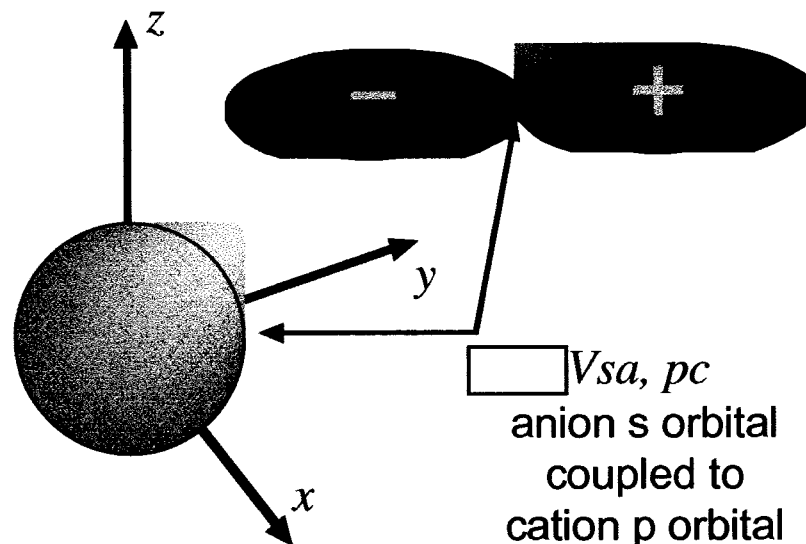
¥ $V_{atomic} = 0 \Rightarrow$ free electron $\Rightarrow E = \frac{\hbar^2}{2m^*} k^2$

Small areas of the Brillouin zone are known experimentally:

¥ Masses / slopes and band edges at symmetry points

¥ Quantitative simulations must reproduce at least the bulk properties!

Fitting $E(k)$ Relations in Tight-Binding

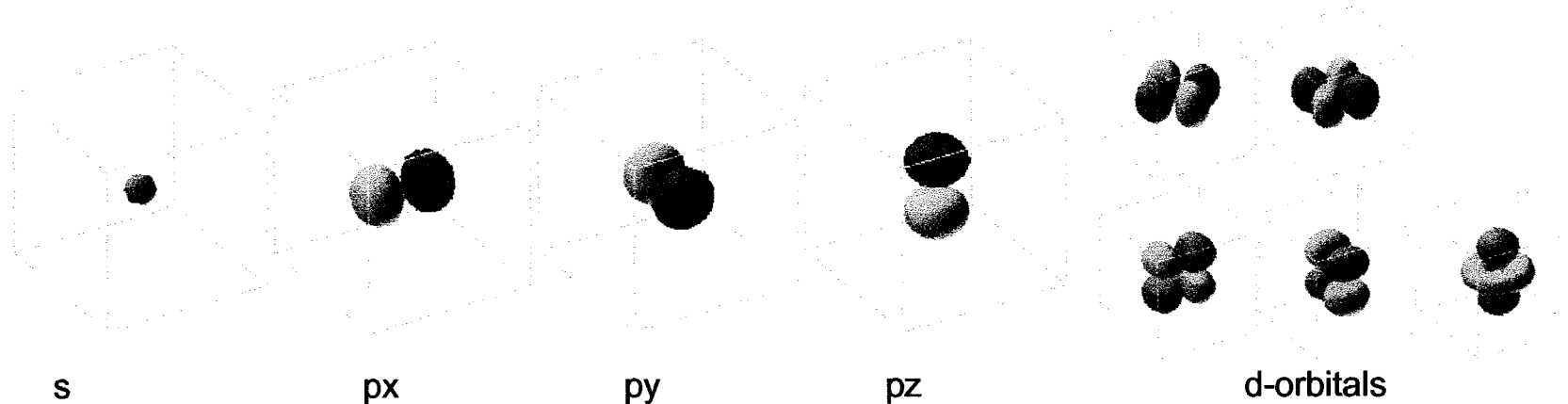


¥Do not have direct control over effective masses and conduction band edges

¥Fit orbital interaction energies

¥Need to choose orbitals and number of neighbors

There are lots of orbitals and lots of neighbors => many interaction energies



sp^3s^* Bandstructure Fitting

¥Open variables - interactions between 10 orbitals on neighboring atoms:

¥13 unconstrained interaction energies

¥2 constrained interaction energies

¥Simulation target:

¥List of 29 physical quantities taken from semiconductor data books

¥Associate a weight / importance with each of these quantities.

¥Minimize error between desired and obtained physical quantities.

¥Population: 3,000

¥Replacement: 5%= 150

¥Generations: 40,000

¥Total # of Genes: 6,003,000

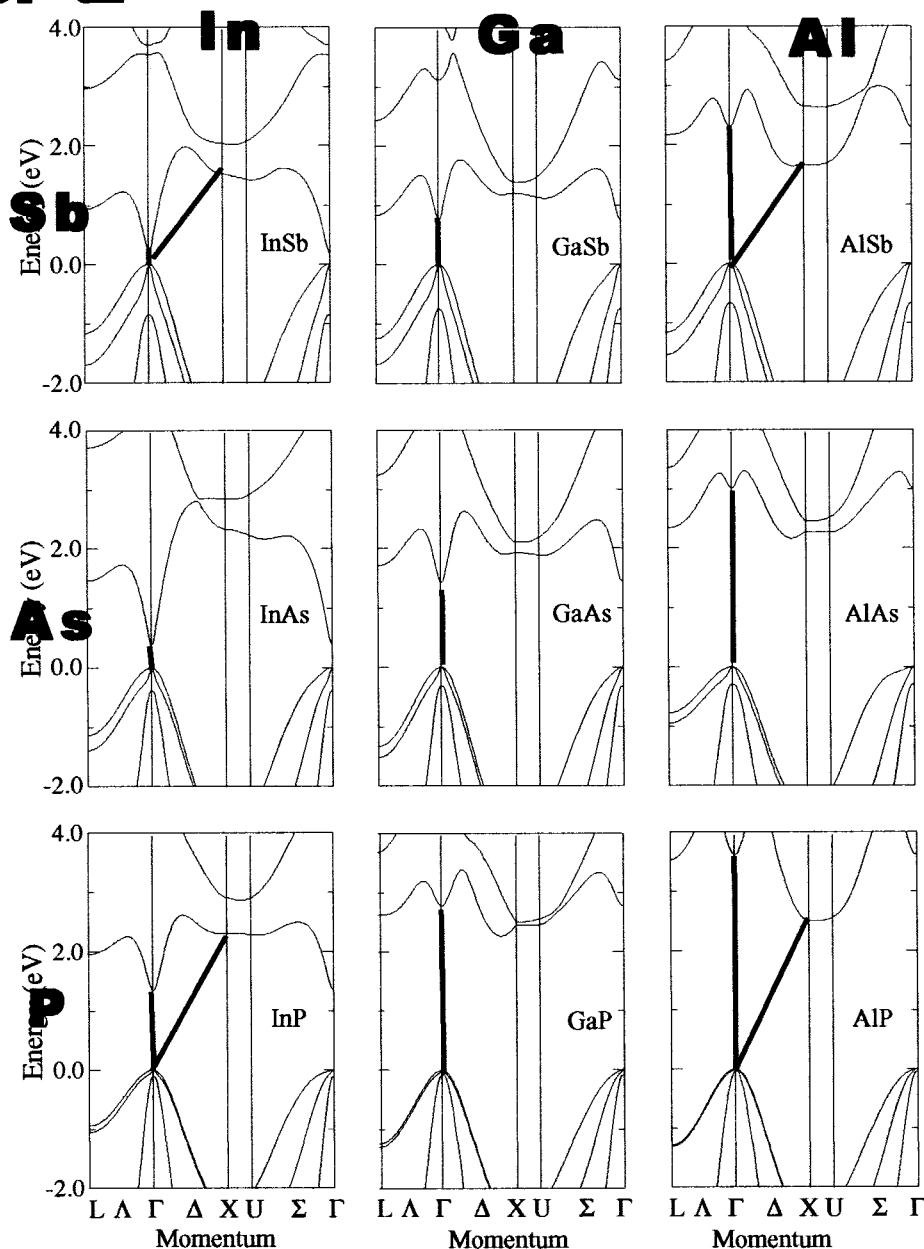
¥Time needed per Gene: 0.5 sec

¥Total time needed: 833hrs for one CPU, 13 hrs for 64 CPUs

¥Compared to derivative based line search:

¥optimization surface is VERY rugged

¥line search gets stuck in nearest local minimum.



Semiconductor Compounds:
cation: In, Ga, Al
anion: Sb, As, P

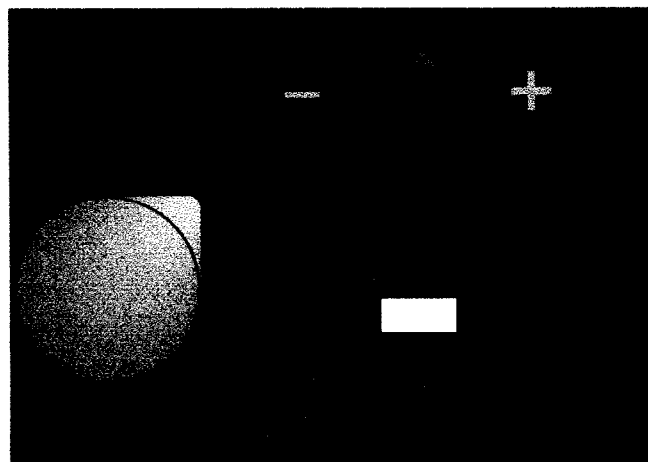
¥Match experimental data in various electron transport areas of the Brillouin zone:

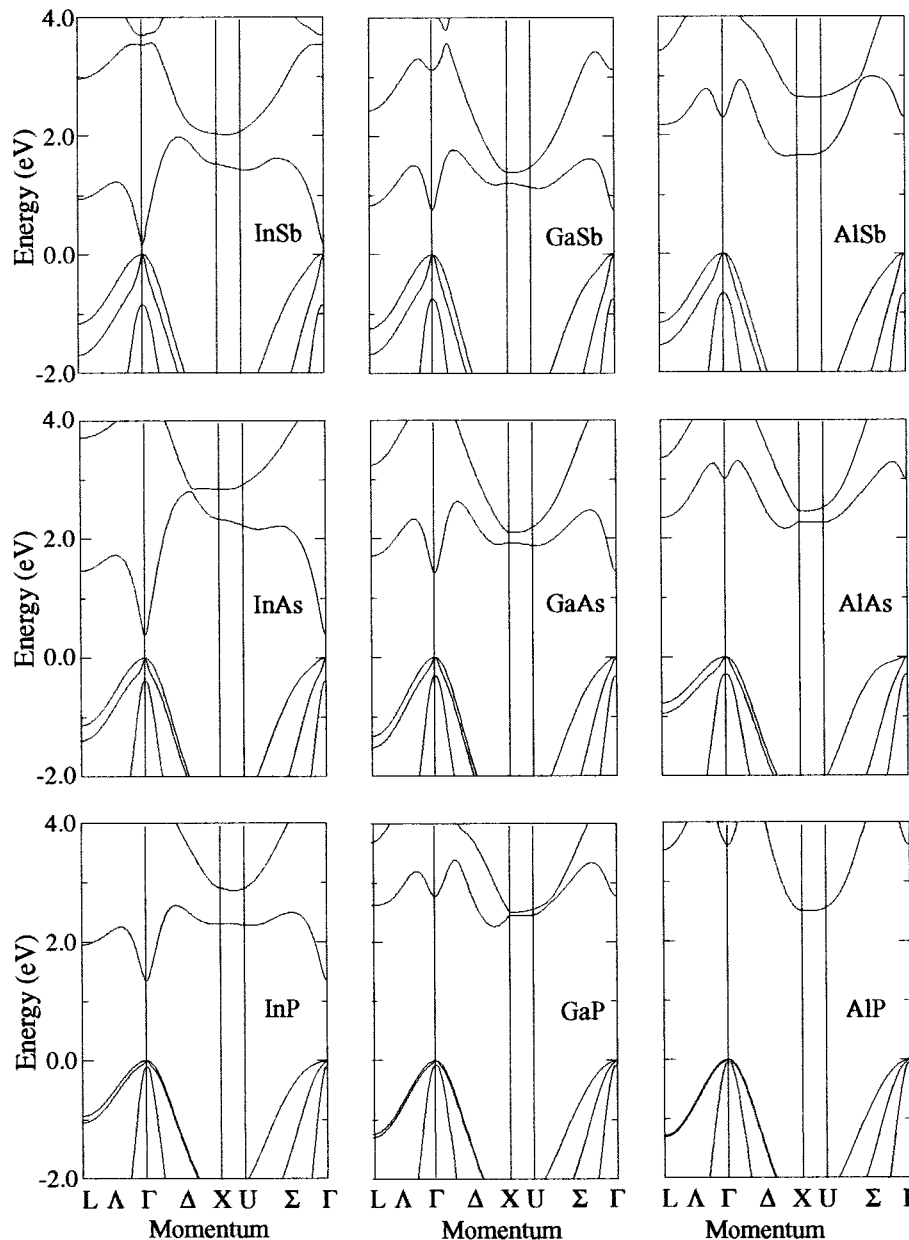
¥Effective masses of electrons at Γ , X and L

¥Effective masses of holes at Γ

¥Band edges at Γ , X and L

¥Each individual material poses a 15 dimensional fitting problem.





Semiconductor Compounds: cation: In, Ga, Al anion: Sb, As, P

¥Match experimental data in various electron transport areas of the Brillouin zone:

¥Effective masses of electrons at Γ , X and L

¥Effective masses of holes at Γ

¥Band edges at Γ , X and L

¥Each individual material poses a 15 dimensional fitting problem.

Next:

¥Treat all materials at once

¥Expl.: In is the same in InSb, InAs, and InP .

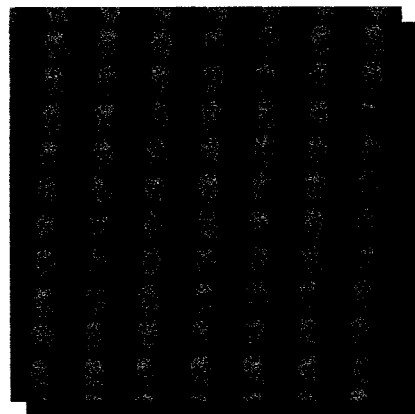
¥6 atoms x 4 on-site energies

¥9 pairs x 7 off-site energies

=> 87 free parameters

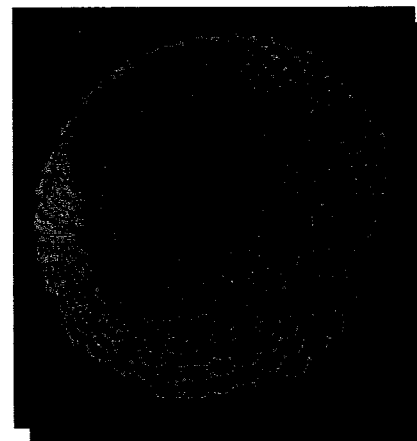
¥Next 2: add more orbitals

Examples of 3D Confined Structures



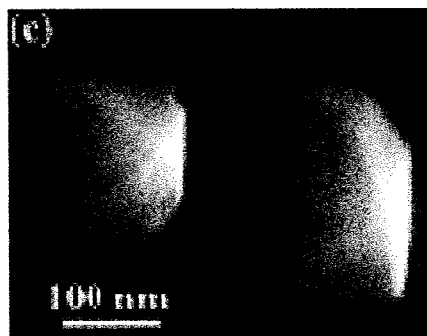
Quantum Dots:
Litho-based,
GaAs/AlGaAs,
InGaAs/InAlAs
systems

Cylinder shaped
M Reed et al, TI
(1988)



Fullerenes, C60:
Carbon based
Electronic and
mechanical appl.

**Rice Univ.,
NASA Ames**

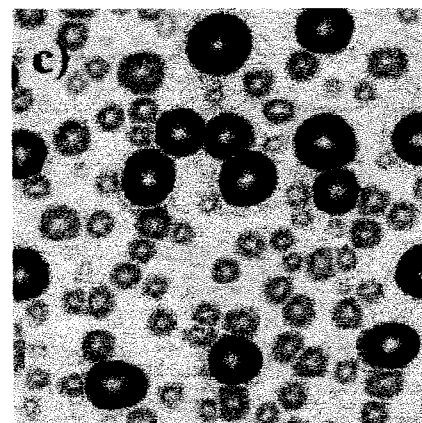


Quantum Dots:
Self-assembled ,
InAs on GaAs.

**Pyramidal or
dome
shaped**



**R. Leon et al,
JPL (1998)**



Quantum Dots:
Self-assembled
Ge on Si.

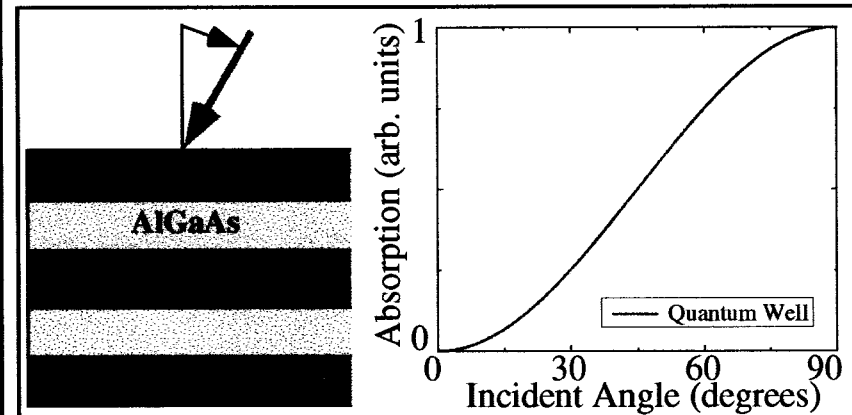
**Dome
shaped**

**S. Williams et al,
HP (1998)**

Quantum Dots as Optical Detectors

Desensitizing QWIP to Polarization

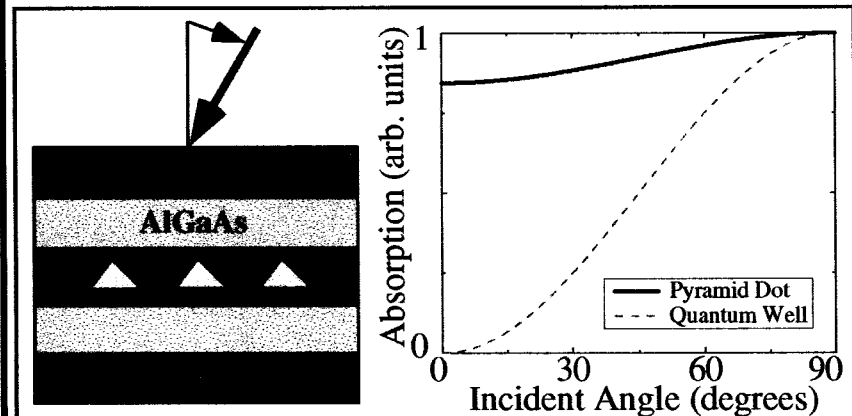
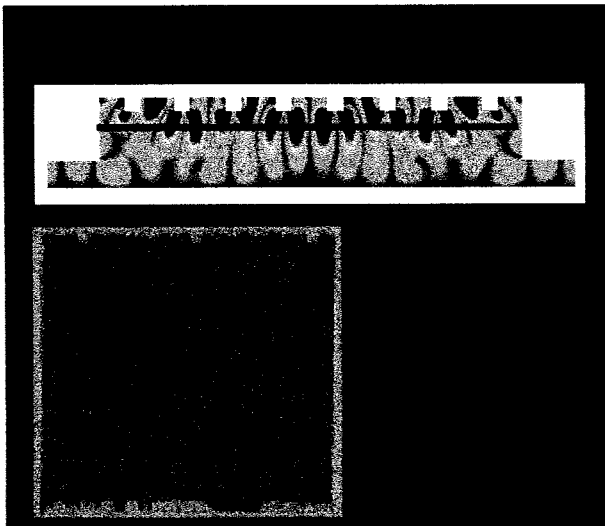
- **Problem:**
Quantum wells are “blind” to light impinging orthogonal to the detector surface.
- **Standard Solution:**
Use gratings to turn polarization
- **New Approach:**
Quantum dots have a built-in anisotropy and state quantization in all three dimensions
-> absorption at all angles



Quantum Wells: Absorption has strong incidence angle dependence

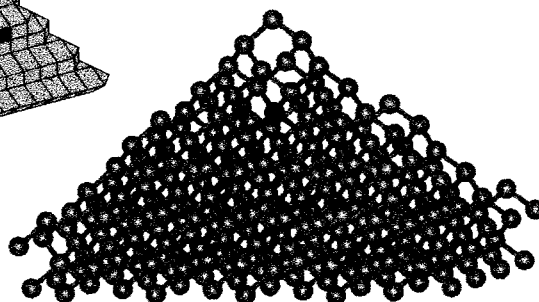
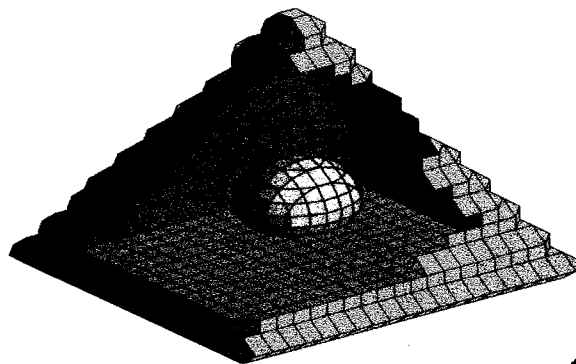
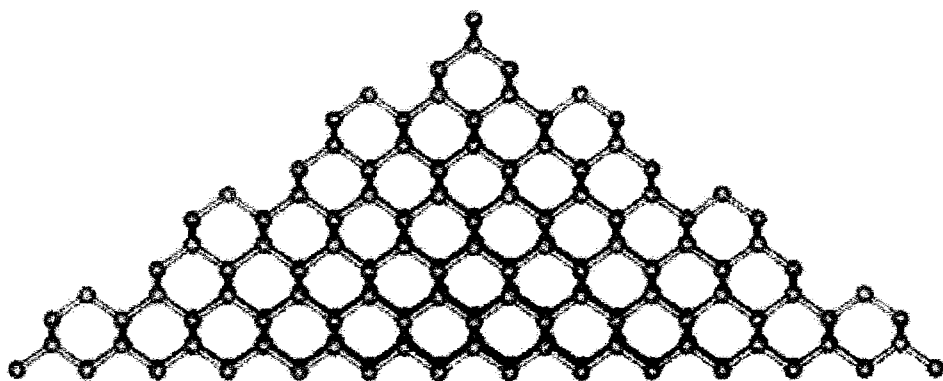
Standard Solution:

Grating



Quantum Dots: Absorption has weak incidence angle dependence

A More Fundamental Problem: How to Represent Materials on an Atomic Scale?



✖ Need to discretize the material on an atomic scale.

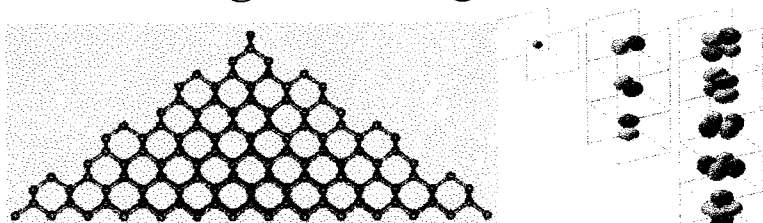
✖ Need to include the crystal symmetry

✖ Need to include the electronic properties of the host atoms:
expl.: Ga, In, As in a InAs/GaAs quantum dot.

✖ Need to get at least the bulk bandstructure right before simulating nanostructures.

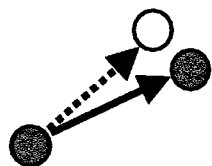
1999 Accomplishments

Atomistic Tight-Binding Hamiltonian

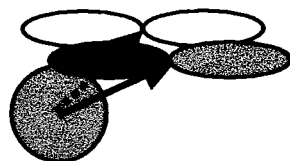


Full crystal symmetry; s,p,d orbitals

Atomistic Strain Model



Atomic locations



Scale bond interactions

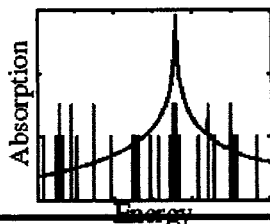
Parallel Lanczos Eigensolver

FLOPS scale $N^{1.1} \Rightarrow 10^6$ Atoms!

GUI: Client Server Tcl/Tk, SQL Database

Optical Interactions

Electric Dipole Transitions
Absorption vs. Energy



2000 Plans

Physics

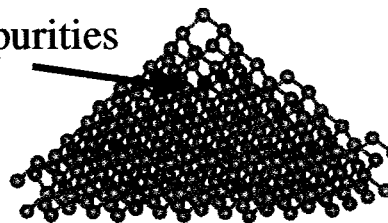
Hartree-Fock potential
Piezo-electric effects
Many-body via configuration interaction
Rate equation based transport

Software

Develop 3D visualization
Shared-memory parallelization (OpenMP)

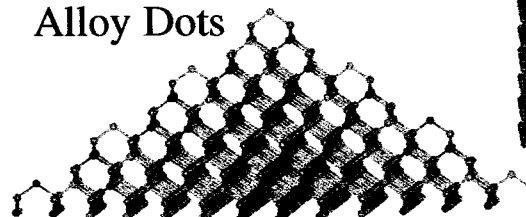
Quantum Dot Simulations

Impurities

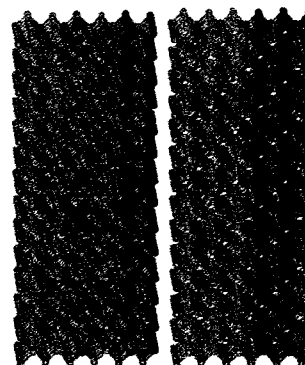


Grading

Alloy Dots



$A_xB_{(1-x)}C$ Dot



Graded

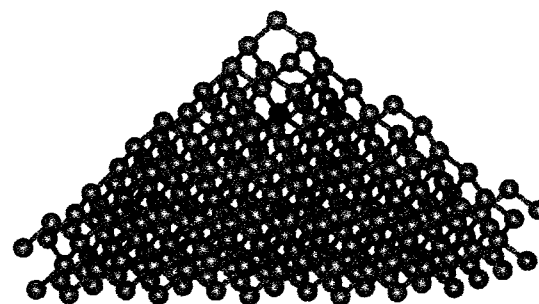
Abrupt

Future Vision

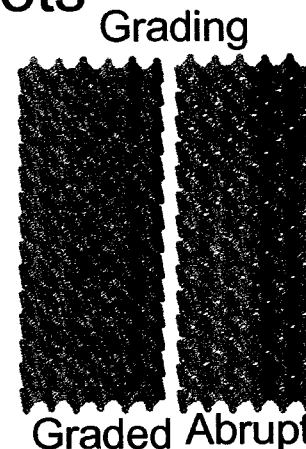
Atomistic Simulation Tool

- ¥ General Structure Input
- ¥ Orbital Basis Extends to Molecules
- ¥ Address CMOS Scaling Issues.

Quantum Dots

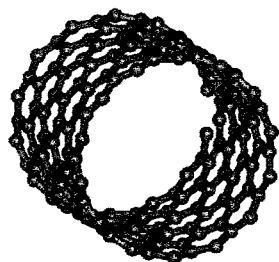


Atomistic Simulation

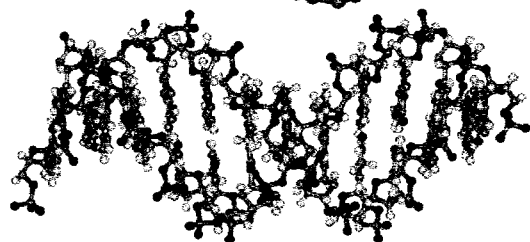


Transport in Molecules

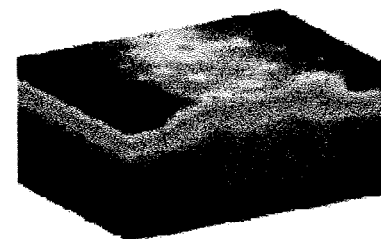
Carbon Nanotubes



DNA



End of SIA Roadmap

Dopant Fluctuations
in Ultra-scaled CMOSElectron Transport
in Exotic Dielectrics